Development of dynamic sub-grid models for variational multiscale methods

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A dynamic Variational Multiscale Method (Hughes *et al.* 1998) is developed by leveraging the Germano procedure from classical Large-eddy Simulations (LES). The similarity between the classical and variational approaches is analyzed in the context of incompressible flow. This analysis leads to a consistent modeling approach for both incompressible and compressible flows, the latter being demonstrated in *a priori* testing for low-speed attached and separated boundary layers. Similar to the classical LES procedure from which it is derived, the variational dynamic procedure does not guarantee a positive semi-definite coefficient in the general case. However, reproducing the behavior of the classical LES dynamic approach is seen as a necessary first step to develop a VMM that automatically adjusts to the local resolution and flow physics.

1. Introduction

The Variational Multiscale Method (VMM) is a reformulation of the classical Large-Eddy Simulations (LES) method, in which the filtering operation, used to explicitly separate resolved and unresolved scales, is replaced by a Galerkin projection operator (Hughes *et al.* 1998, 2000). The long-distance triadic interactions involving the unresolved scales are ignored. The unresolved scales are assumed to only interact with the finest resolved scales, thus ensuring that no energy is removed from the large structures in the flow *via* a model.

Previous work using VMM demonstrates the success of using a fixed-coefficient eddy-viscosity model for the sub-grid stresses, including for attached wall-bounded applications (Hughes *et al.* 2000, 2001, 2004; Bazilevs *et al.* 2007). In order to apply the method to general complex flows, including those with separation, it is necessary to replace the fixed-coefficient model with a mechanism that automatically adapts to the local resolution and flow physics. As the typical VMM model is based on a Smagorinsky eddy-viscosity model, leveraging Germano's dynamic procedure from classical LES (Germano *et al.* 1991) is an obvious first step. This has been accomplished for finite-volume schemes using an agglomeration operator developed by Farhat *et al.* (2006) to separate the fine and coarse scales.

The current work develops a dynamic VMM approach for an entropy-stable Discontinuous-Galerkin spectral-element solver (Diosady & Murman 2013, 2014). The use of spectral elements provides an efficient scheme for resolving complex flows with a range of physical scales, and also a method that provides clear separation of these scales for the VMM.

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2. Dynamic Eddy-viscosity Model

Here we develop a dynamic compressible VMM formulation. However, we begin by describing the dynamic approach for the incompressible Navier-Stokes equations to simplify the discussion, highlight the similarities to the classical LES approach, and demonstrate the parallels to the compressible formulation. Development of an entropy-stable compressible formulation then follows in the next section.

The incompressible, isothermal Navier-Stokes equations are given by

$$u_{i,i} = 0 \tag{2.1}$$

$$u_{i,t} + \left(u_i u_j\right)_{,j} = -\frac{1}{\rho}\partial_j\left(p\delta_{ij}\right) + \nu u_{i,jj}, \tag{2.2}$$

where the comma indicates partial differentiation. Writing the momentum equations in weak form over the domain Ω we have

$$\begin{aligned} &\left(u_{i,t}, w_i\right) - \left(u_i u_j, w_{i,j}\right) - \frac{1}{\rho}\left(p\delta_{ij}, w_{i,j}\right) + \left(\nu u_{i,j}, w_{i,j}\right) \\ &+ \left(u_i u_j + p\delta_{ij}, w_i n_j\right)_{\partial\Omega} - \left(\nu u_{i,j}, w_i n_j\right)_{\partial\Omega} = 0 \quad \forall w \in \mathcal{V}, \end{aligned} \tag{2.3}$$

where w is the test function. This is written compactly as

$$R_u\left(u, w\right) = 0. \tag{2.4}$$

where R_u is the bilinear operator of Eqn. 2.3.

In a variational multiscale method we *a priori* decompose the continuous space as $\mathcal{V} = \tilde{\mathcal{V}} \cup \check{\mathcal{V}} \cup \hat{\mathcal{V}}$ where $\tilde{\mathcal{V}}$ are the coarse scales, $\check{\mathcal{V}}$ are the fine scales, and $\hat{\mathcal{V}}$ are the unresolved scales that cannot be represented on the current discretization (*cf.* Fig. 1, Collis (2001)). A similar decomposition follows for the velocity field, $u = \tilde{u} + \check{u} + \hat{u}$. Under suitable choice of orthogonal spaces, $\tilde{\mathcal{V}} \cap \check{\mathcal{V}} = \emptyset$, *etc.*, we have the following for the incompressible momentum equations

$$R_u\left(\bar{u}, \bar{w}\right) + \tau\left(u, \bar{w}\right) = 0 \quad \forall \bar{w} \in \bar{\mathcal{V}} = \tilde{\mathcal{V}} \cup \check{\mathcal{V}}, \tag{2.5}$$

where $\bar{u} = \tilde{u} + \check{u}$, $\bar{w} = \tilde{w} + \check{w}$, and

$$\tau\left(u, \bar{w}\right) = \left(\hat{u}_i\hat{u}_j, \bar{w}_{i,j}\right) + \left(\bar{u}_i\hat{u}_j, \bar{w}_{i,j}\right) + \left(\hat{u}_i\bar{u}_j, \bar{w}_{i,j}\right) \tag{2.6}$$

$$= \left(u_i u_j - \bar{u}_i\bar{u}_j, \bar{w}_{i,j}\right) \tag{2.7}$$

is the projection of the unresolved/"subgrid-scale" stress terms onto $\bar{w}$ that must be modeled to close the system.

The VMM assumes the unresolved scales only interact with the fine scales. The coarse and fine scales are defined by low-pass ($\mathbb{P}$) and high-pass ($\overline{\mathbb{P}}$) orthogonal projection operators respectively on the resolved scales,

$$\tilde{w} = \mathbb{P}\bar{w}, \quad \check{w} = \overline{\mathbb{P}}\bar{w}, \quad \overline{\mathbb{P}}\left(\mathbb{P}\bar{w}\right) = \emptyset, \quad \mathbb{P}\left(\overline{\mathbb{P}}\bar{w}\right) = \emptyset. \tag{2.8}$$

Assuming a gradient-diffusion (eddy-viscosity) model for τ we have

$$\tau\left(u, \bar{w}\right) \simeq -2\left(\left(C_1\Delta\right)^2 \|\check{S}_{i,j}\|\check{S}_{i,j}, \check{w}_{i,j}\right), \tag{2.9}$$

where $S_{i,j} = 1/2\left(u_{i,j} + u_{j,i}\right)$ is the symmetric strain-rate tensor. This is similar to the high-pass filtered Smagorinsky models (*cf.* Stolz *et al.* 2004). The subgrid-stress coefficient C_1 is not equivalent to the standard Smagorinsky constant due to the scale

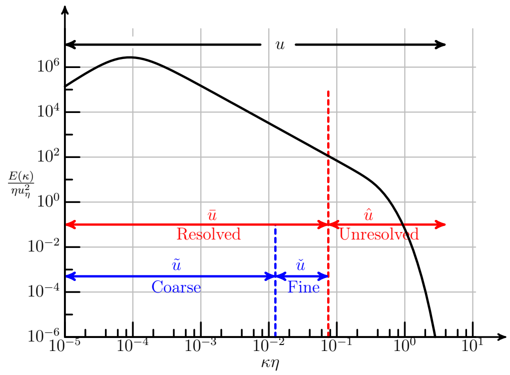

FIGURE 1. *A priori* scale separation for a variational multiscale method following the triple decomposition of Collis (2001).

separation of the VMM. The subgrid-stress coefficient is inside the inner product operator, which is akin to keeping the Smagorinsky constant inside the filter operator in a classical LES method.

Equation 2.9 is a bilinear operator valid over any space $\bar{\mathcal{V}}$, hence we can construct a variational analogue to the classical LES Germano dynamic procedure (Germano *et al.* 1991) to determine the eddy-viscosity coefficient. Denoting the current resolution by h, and applying a second projection (filter) operator to a coarser "test" space, H, we have the subgrid-stress on the current and test space as

$$\tau\left(u, \bar{w}^h\right) = \left(u_i u_j - \bar{u}_i^h \bar{u}_j^h, \bar{w}_{i,j}^h\right) \tag{2.10}$$

$$T\left(u, \bar{w}^H\right) = \left(u_i u_j - \bar{u}_i^H \bar{u}_j^H, \bar{w}_{i,j}^H\right). \tag{2.11}$$

Projecting the subgrid-stresses τ to the test space H and forming the variational dynamic Leonard stresses gives

$$\begin{aligned} L\left(u, \bar{w}^H\right) = T\left(u, \bar{w}^H\right) - \tau\left(u, \bar{w}^H\right) = \left(\bar{u}_i^h \bar{u}_j^h - \bar{u}_i^H \bar{u}_j^H, \bar{w}_{i,j}^H\right) = \\ -2\left(\left(C_1 \Delta\right)^2 \|\check{S}_{i,j}^h\| \check{S}_{i,j}^h, \check{w}_{i,j}^H\right) + 2\left(\left(C_1 \Delta\right)^2 \|\check{S}_{i,j}^H\| \check{S}_{i,j}^H, \check{w}_{i,j}^H\right), \end{aligned} \tag{2.12}$$

where we've likewise followed a similar procedure for the modeled subgrid-stresses. Note that this approach varies from the dynamic localization of Ghosal *et al.* (1995), whereby a variational formulation is built from the strong form of the Leonard stresses. Here a consistent formulation is used to directly construct a dynamic procedure for the variational form of the subgrid model stresses, similar to the approaches of Oberai & Wanderer (2006) and Farhat *et al.* (2006).

Because the VMM modeling assumption only includes the fine scales, while the subgrid stress includes all scales, Eqn. 2.12 cannot be satisfied exactly for any coefficient C_1. By choosing a particular basis for the test space, Eqn. 2.12 becomes an over-determined matrix system which can be solved in a least-squares sense to determine C_1, which could then potentially vary in space and time within an element depending upon the dimensions of the fine space, test space, *etc.* The difficulty with this approach is that the solution to this matrix system is dependent upon the space $\bar{\mathcal{V}}^H$, which is arbitrary, unlike the solution to the Galerkin form of the equations which is independent of the choice of basis. For example, even maintaining the same linear span, but performing a translation of the

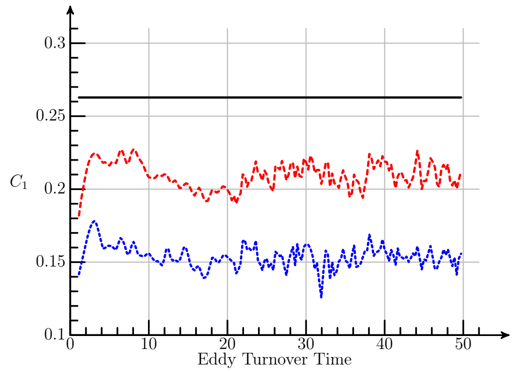

FIGURE 2. *A priori* testing of the subgrid stress modeling assumptions for forced homogeneous isotropic turbulence at $Re_\lambda = 300$. —— Kolmogorov ($C_S = 0.18$) , - - - - Germano , - - - - Lilly

basis will produce a different coefficient C_1. Philosophically, the least-squares approach to Eqn. 2.12 is purely a linear algebra solution, and does not take advantage of available physical insight. Thus, the preferred approach here is to choose an appropriate subspace of $\bar{\mathcal{V}}^H$ in conjunction with the VMM model approximation which does provide physical insight.

If C_1 is assumed constant within an element, the inner product can be used to reduce Eqn. 2.12 to a scalar equation with clear physical interpretation. For example, using the velocity as the test function, $\bar{w}_{i,j} = \bar{u}_{i,j}$, produces a variational analogue to Germano's dynamic procedure for classical LES. Similarly, defining

$$M_{ij} = -2\Delta^2 \|\check{S}^h_{i,j}\| \check{S}^h_{i,j} + 2\Delta^2 \|\check{S}^H_{i,j}\| \check{S}^H_{i,j} \tag{2.13}$$

and using the L_2 projection of M_{ij} for the test function reproduces a variational analogue of Lilly's least-square procedure (Lilly 1991).

2.1. *Homogeneous Isotropic Turbulence*

A priori testing of the subgrid stress modeling assumptions using Direct Numerical Simulation (DNS) data is performed for forced homogeneous isotropic turbulence at $Re_\lambda = 300$. The ideal LES velocity field is constructed by low-pass filtering the DNS so that the highest resolved wavenumber $\kappa\eta \leq 0.1$. Figure 2 presents the variation of C_1 within the domain using the variational analogue to the Germano and Lilly procedures, along with the model spectrum assuming Kolmogorov's -5/3 law for the inertial range. The latter is considered an upper bound for the coefficient. In this experiment $\bar{k}^H/\bar{k}^h = 2/3$ and $\tilde{k}^h/\bar{k}^h = \tilde{k}^H/\bar{k}^H = 1/2$, where k is the magnitude of the spectral wave number. After an initial transient both models achieve a statistically-stationary positive correlation, with the Germano procedure producing the larger eddy-viscosity coefficient.

The behavior in Fig. 2 can be understood more thoroughly by examining the individual terms in the dynamic Germano procedure. Using $\bar{w}_{i,j} = \bar{u}_{i,j}$, the test scale dissipation is

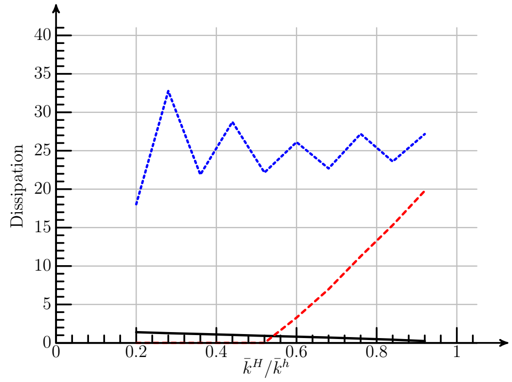

FIGURE 3. *A priori* testing of the subgrid stress modeling assumptions in the variational Germano procedure for forced homogeneous isotropic turbulence at $Re_\lambda = 300$. —— $\left(\bar{u}_i^h \bar{u}_j^h, \bar{u}_{i,j}^H\right)$, - - - - $-2\left((C_1\Delta)^2 \|\check{S}_{i,j}^h\| \check{S}_{i,j}^h, \check{S}_{i,j}^H\right)$, - - - - $-2\left((C_1\Delta)^2 \|\check{S}_{i,j}^H\| \check{S}_{i,j}^H, \check{S}_{i,j}^H\right)$

given by

$$\left(\bar{u}_i^H \bar{u}_j^H, \bar{u}_{i,j}^H\right) = \int_\Omega \bar{u}_i^H \bar{u}_i^H \bar{u}_{j,j}^H + \bar{u}_j^H \partial_j \left(\frac{\bar{u}_i^H \bar{u}_i^H}{2}\right) = 0 \tag{2.14}$$

for the periodic domain. Similarly, the modeled subgrid-stress dissipation for the resolved scale is given by

$$-2\left((C_1\Delta)^2 \|\check{S}_{i,j}^h\| \check{S}_{i,j}^h, \check{w}_{i,j}^H\right) = -2\left((C_1\Delta)^2 \|\check{S}_{i,j}^h\| \check{S}_{i,j}^h, \check{S}_{i,j}^H\right). \tag{2.15}$$

If $\check{\mathcal{V}}^H \cap \check{\mathcal{V}}^h = \emptyset$, then this term is zero. Lastly, using the Kolmogorov model spectrum, the modeled subgrid-stress dissipation for the test scale is independent of the ratio of the test scale to the resolved scale.

The variation of each of the subgrid-stress dissipation terms with ratio of test scale to resolved scale, $\bar{k}^H/\bar{k}^h$, is given in Fig. 3 for the dynamic Germano procedure. This data is averaged over 30 eddy turnover times. The modeled subgrid-stress dissipation for the test scale is roughly a constant, while the projections from the resolved scale to the test scale both vary linearly. From this, it is determined that the subgrid-stress coefficient C_1 is independent of the ratio $\bar{k}^H/\bar{k}^h$ for this flow provided $\check{\mathcal{V}}^H \cap \check{\mathcal{V}}^h \neq \emptyset$, which requires the minimum a 4th-order spectral element. The Lilly procedure does not share this property.

3. Compressible Formulation

The Navier-Stokes equations for compressible viscous flow are

$$q_{i,t} + f_{ij,j} - g_{ij,j} = 0, \tag{3.1}$$

where q_i are the conserved quantities, f_{ij} is the inviscid flux, and g_{ij} is the viscous flux,

$$q_i = \begin{pmatrix} \rho \\ \rho u_k \\ \rho e \end{pmatrix}, \quad f_{ij} = \begin{pmatrix} \rho u_j \\ \rho u_k u_j + p\delta_{kj} \\ \rho e u_j + p u_j \end{pmatrix}, \quad g_{ij} = \begin{pmatrix} 0 \\ \tau_{kj} \\ u_k \tau_{kj} + \kappa T_{,j} \end{pmatrix}.$$

Writing Eqn. 3.1 in weak form gives

$$(q_{i,t}, w_i) - (f_{ij}, w_{i,j}) + (g_{ij}, w_{i,j}) + (f_{ij}, w_i n_j)_{\partial\Omega} - (g_{i,j}, w_i n_j)_{\partial\Omega} = 0 \quad \forall w \in \mathcal{V} \tag{3.2}$$

or

$$R_q(q, w) = 0 \quad \forall w \in \mathcal{V}. \tag{3.3}$$

Again decomposing into fine, coarse, and unresolved scales, we assume that the effect of the unresolved scales on the diffusion coefficients is negligible. This gives

$$R_q(\bar{q}, \bar{w}) + \beta(q, \bar{w}) = 0 \quad \forall \bar{w} \in \bar{\mathcal{V}}, \tag{3.4}$$

where

$$\beta(q, \bar{w}) = (f_{ij}(q) - f_{ij}(\bar{q}), \bar{w}_{i,j}). \tag{3.5}$$

Introducing the generalized entropy variables that symmetrize the compressible Navier-Stokes equations (*cf.* Hughes *et al.* 1986, Barth 1999),

$$v_i = \begin{pmatrix} -\frac{s}{\gamma-1} + \frac{\gamma+1}{\gamma-1} - \frac{\rho e}{p} \\ \frac{\rho u_k}{p} \\ -\frac{\rho}{p} \end{pmatrix}, \tag{3.6}$$

we then have

$$\beta(v, \bar{w}) \simeq (f_{ij}(v) - f_{ij}(\bar{v}), \bar{w}_{i,j}). \tag{3.7}$$

Numerically, entropy in compressible flow fills an analogous (though more complex) role to kinetic energy in incompressible flow. When simulating an incompressible flow we desire a scheme with a global energy bound, whereas in compressible flow simulations we desire a scheme with a global entropy bound. As seen above in Eqn. 2.14, the momentum flux is an advection of kinetic energy when the velocity field is used as the test function. Analogously, choosing the entropy variables as the test function in Eqn. 3.7 leads to advection of entropy for the resolved "stresses",

$$(f_{ij}, v_{i,j}) = \int_\Omega \partial_i(u_i \rho s) = \int_{\partial\Omega} \rho s u_i n_i \quad \text{compressible} \tag{3.8}$$

$$(u_i u_j, u_{j,i}) = \int_\Omega \partial_i \left(u_i \frac{u_j u_j}{2}\right) = \int_{\partial\Omega} \frac{u_j u_j}{2} u_i n_i \quad \text{incompressible} \tag{3.9}$$

Because the entropy variables are complex nonlinear functions of the conservative variables, the model integrated using entropy variables is not identical to the scale separation in conservative variables, *i.e.* $f_{ij}(\bar{v}) \neq f_{ij}(\bar{q})$. A similar approximation under different modeling assumptions is described in Leveasseur *et al.* (2006). The alternative, applying the scale separation directly to the entropy variables, introduces nonlinear products in the time derivative that are difficult to model. In the current low-speed numerical tests these approximations are unimportant. A more thorough analysis of the modeling assumptions for high-speed compressible flow is left for future work.

The subgrid-stress model for compressible flows mimics the diffusion terms in entropy

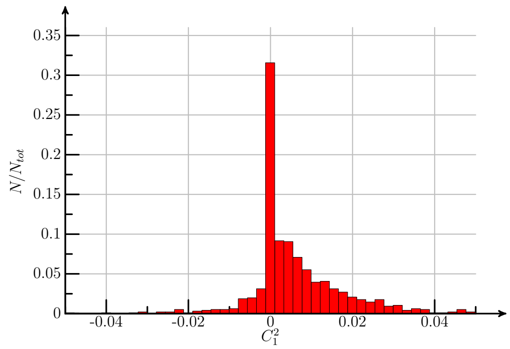

FIGURE 4. Histogram of instantaneous subgrid-stress coefficient for planar channel flow at $Re_\tau = 180$.

variables,

$$\beta\left(v,\bar{w}\right) \simeq -\left(\left(C_1\Delta\right)^2 \|\check{v}_{i,j}\|\check{v}_{i,j}, \check{w}_{i,j}\right). \tag{3.10}$$

The dynamic procedure then becomes

$$\left(f_{ij}\left(\bar{v}^h\right) - f_{ij}\left(\bar{v}^H\right), \bar{w}^H_{i,j}\right) = -\left(\left(C_1\Delta\right)^2 \|\check{v}^h_{i,j}\|\check{v}^h_{i,j}, \check{w}^H_{i,j}\right) + \left(\left(C_1\Delta\right)^2 \|\check{v}^H_{i,j}\|\check{v}^H_{i,j}, \check{w}^H_{i,j}\right), \tag{3.11}$$

with the entropy variables used as the test function to determine the scalar coefficient C_1. Alternatively, by assuming a value for the subgrid-stress Prandtl number the modeled stresses can be constructed using the subgrid-stress analogue to the full viscous Jacobian instead of the diagonal approximation in Eqn. 3.10. These two approaches are indistinguishable in the current low-speed testing.

3.1. A priori *Testing*

The behavior of the dynamic VMM subgrid-model is investigated using two DNS databases computed in Diosady & Murman (2014) - channel flow at $Re_\tau = 180$, and separated flow over an array of hills. In both cases, the LES field is constructed by coarsening by a factor of two in both h and p. Unlike the numerical tests in Sec. 2.1, here the local finite elements do not span the entire domain. This introduces the difficulty that the subgrid-stress coefficient is no longer guaranteed to be positive semi-definite. This is not surprising, as the current approach leverages the dynamic procedure from classical LES - both the positive and negative aspects. Examining Eqn. 3.11, the difficulty is the projection of the flux to the test level. As this is related to an advection of entropy when $\bar{w}^H_{,j} = \bar{v}^H_{i,j}$, eddy structures that are larger than the finite element size will locally advect subgrid entropy from an element at a greater rate than it is produced, while in neighboring elements the opposite is true. Figure 4 presents a histogram of C_1 at one instant in time for all of the elements in the three-dimensional channel flow simulation. Although the mean is positive, many elements at any instant have a negative subgrid-stress coefficient as the difference $\left(f_{ij}\left(\bar{v}^h\right) - f_{ij}\left(\bar{v}^H\right), \bar{v}^H_{i,j}\right)$ is negative.

A common technique in classical LES is averaging the instantaneous coefficient over homogeneous directions. In the case of fully developed channel flow, this includes the streamwise and spanwise directions. In the current variational context, the net advection of entropy is zero in the homogeneous directions, hence this filters some of the large-scale eddy motion at each time sample. The large-scale motions in the wall-normal directions

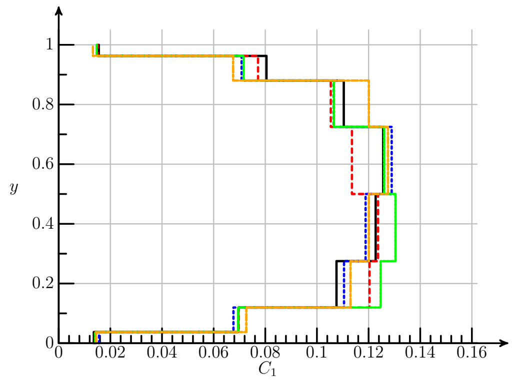

FIGURE 5. Subgrid-stress coefficient averaged over the homogeneous directions at five time samples for planar channel flow at $Re_\tau = 180$. —— $t_e = 22$, - - - - $t_e = 22.16$, - - - - $t_e = 22.33$, ······· $t_e = 22.5$, ········· $t_e = 22.67$

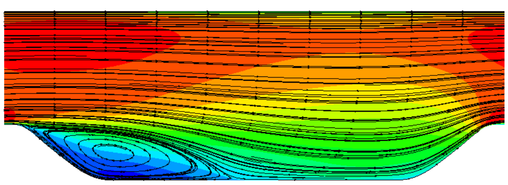

FIGURE 6. Mean streamlines for flow over an array of hills.

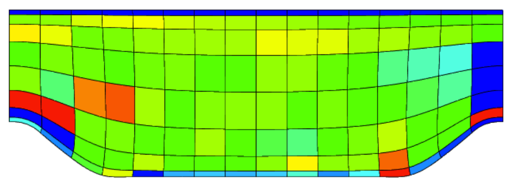

FIGURE 7. Spatial variation of the spanwise-averaged subgrid-stress coefficient for flow over an array of hills. Blue is zero and red is 0.1.

are constrained near the wall, limiting the magnitude of the advection in this direction. The subgrid-stress coefficient averaged over the homogeneous directions is plotted in Fig. 5 for 5 time samples. There are 8 elements in the wall-normal direction, and the coefficient is constant within each element, and discontinuous between elements. The peak coefficient is roughly half the value of the coefficient for homogeneous isotropic turbulence, which is physically plausible. The coefficient also approaches zero at the top and bottom walls of the channel as desired. There is greater variation in time near the center of the channel, where there are correspondingly larger eddy structures.

The final example presents the mean dynamic coefficient for the separated flow over an array of hills (Figs. 6 & 7). In this case only the spanwise direction is homogeneous, leaving both large-scale motions in the streamwise direction and thin separated shear layer in the center of the channel which cause difficulty for the dynamic procedure. The instantaneous subgrid-scale coefficient does become negative in some elements even when averaging over the spanwise direction. Outside this separated flow near the apex of the hill, the variation of the coefficient on the upper wall is essentially identical to the channel flow results, and a small positive value of the coefficient is produced in the recirculation region.

4. Summary

A variational analogue to the classical Germano dynamic procedure from classical LES has been used to develop a dynamic VMM for incompressible and compressible flows. *A priori* testing demonstrates that this methodology provides physically plausible values of the subgrid-stress coefficient for several benchmark flows. Next, *a posteriori* testing of the model predictions on similar benchmark flows will be used to refine the approach.

Acknowledgments

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